1-Methylpyrene

2381-21-7 | DTXSID0025654

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.16e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.03e-01

Confidence level: 5.24e-01

Nearest Neighbors from the Training Set

Image not found
1,4-Diaminoanthraquinone
Measured: 4.50e-06
Predicted: 7.81e-10

Image not found
Benzo(b)fluoranthene
Measured: 9.22e-06
Predicted: 9.46e-09

Image not found
11H-Benzo[a]fluorene
Measured: 5.50e-08
Predicted: 2.19e-07

Image not found
Benzo[h]quinoline
Measured: 2.43e-07
Predicted: 1.01e-04

Image not found
1,1':3',1"-Terphenyl
Measured: 2.49e-09
Predicted: 9.36e-06